The color of X-rays

Enrico Junior Schioppa

DPNC UNIGE
CTA/IceCube
THE COLOR OF X-RAYS

Spectral X-ray computed tomography using energy sensitive pixel detectors

ACADEMISCH PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Universiteit van Amsterdam op gezag van de Rector Magnificus prof. dr. D.C. van den Boom
ten overstaan van een door het college voor promoties ingestelde commissie, in het openbaar te verdedigen in de Aula der Universiteit

Promotiecommissie:

Promotor: prof. dr. ir. E.N. Koffeman
Co-promotor: dr. J. Visser
Overige Leden: prof. dr. S.C.M. Bentvelsen
dr. A.P. Colijn

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X-ray imaging: how it all started

- X-rays absorbed in the hand
- Count how many “survive”
Very short history of X-ray imaging

1896 Radiography Dual energy Computed Tomography (CT)

Resolution ~ 0.1-0.2 mm at best (cannot focus X-rays!)
Interaction of photons with matter

X-ray range  Photoelectric effect
All energy released!
It's all a matter of survival chance

Number of zebras that DON'T make it

• Number of zebras
• Distance
• Dangerousness
Photon attenuation

$$I = I_0 - \Delta I$$
Photon attenuation

Photon attenuation is described by the following equations:

\[ I = I_0 - \Delta I \]

\[ \delta I = -\mu I \delta s \]

where \( I_0 \) is the initial intensity, \( I \) is the intensity after attenuation, \( \Delta I \) is the change in intensity, \( \mu \) is the attenuation coefficient, and \( \delta s \) is the distance over which the attenuation occurs. The attenuation coefficient \( [\mu] \) is measured in units of \( s^{-1} \).
Photon attenuation

\[ I_0 \quad \mu \quad I = I_0 - \Delta I \]

\[ \delta I = -\mu I \delta s \]

\[ [\mu] = [s^{-1}] \]

\[ I = I_0 e^{-\mu s} \]
Integral along a ray path

\[ \mu(x, y) \rightarrow \mu(s) \]
Integral along a ray path

\[ I_{l, \theta} = I_0 e^{-\int_{l, \theta} \mu(s) \, ds} \]

where \( \mu(x, y) \rightarrow \mu(s) \).
Sinograms

The sinogram contains information about the object slice.
Quick introduction to Computed Tomography (CT)
The CT image reconstruction problem

Set of X-ray images at different angles

3D image
CT reconstruction as a set of linear equations

\[ I_{l, \theta} = I_0 e^{-\int_{l, \theta} \mu(s) ds} \]

\[ \int_{l, \theta} \mu(s) ds = -\log \frac{I_{l, \theta}}{I_0} \]
CT reconstruction as a set of linear equations

\[ I_{l, \theta} = I_0 e^{-\int_{l, \theta} \mu(s) \, ds} \]

\[ \int_{l, \theta} \mu(s) \, ds = -\log \frac{I_{l, \theta}}{I_0} \]
CT reconstruction as a set of linear equations

\[ I_{l, \theta} = I_0 e^{-\int_{l, \theta} \mu(s) ds} \]

\[ \int_{l, \theta} \mu(s) ds = -\log \frac{I_{l, \theta}}{I_0} \]

\[ I_0 e^{-\int_{l, \theta} \mu(s) ds} = I_{l, \theta} \]
CT reconstruction as a set of linear equations

\[ I_{l, \theta} = I_0 e^{-\int_{l, \theta} \mu(s) ds} \]

\[ \int_{l, \theta} \mu(s) ds = -\log \frac{I_{l, \theta}}{I_0} \]

\[ I_0(E) e^{-\int_{l, \theta} \mu(s, E) ds} = I_{l, \theta}(E) \]
Monochromatic X-ray sources?

Monochromators?

Synchrotrons?

Impractical!
The real CT equations

\[ I_0(E) \]
The real CT equations

\[ I_0(E) e^{-\int_{l, \theta} \mu(s, E) ds} \]
The real CT equations

\[ \int_{0}^{+\infty} dE \, R(E; E') \, I_0(E) \, e^{-\int_{l, \theta} \mu(s, E) \, ds} \]

detector response function

Probability that a photon at energy \( E \) is detected as having energy \( E' \)

attenuation curves

source spectrum
The real CT equations

\[ N_{l, \theta} = \int_0^{+\infty} dE' \int_0^{+\infty} dE R(E; E') I_0(E) e^{-\int_{l, \theta} \mu(s, E) ds} \]

Probability that a photon at energy \( E \) is detected as having energy \( E' \)

One number!
Principle of conventional X-ray detection

Charge ↔ energy
Principle of conventional X-ray detection

Charge ↔ energy
Some brain missing?

What the heck is going on here?

Image artifacts in CT

Parameters of electromagnetic radiation

An electromagnetic wave
Material decomposition

\[ N_{l, \theta} = \int_0^{+\infty} \ldots e^{-\int_{l, \theta} \mu(s, E) \, ds} \]

Not linear, but this is the only equation we have
Material decomposition

\[ N_{l, \theta} = \int_{0}^{+\infty} e^{-\int_{l, \theta}^{\infty} \mu(s, E) \, ds} \]

\[ N_{l, \theta} = \int_{0}^{+\infty} e^{-\int_{l, \theta}^{\infty} [\alpha_1 \mu_1(s, E) + \alpha_2 \mu_2(s, E)] \, ds} \]

Not linear, but this is the only equation we have.
Material decomposition

\[ N_{l, \theta} = \int_{0}^{+\infty} \ldots e^{-\int_{t, \theta} \mu(s, E) \, ds} \]

Not linear, but this is the only equation we have

\[ N_{l, \theta} = \int_{0}^{+\infty} \ldots e^{-\int_{t, \theta} [\alpha_1 u_1(s, E) + \alpha_2 u_2(s, E)] \, ds} \]

\[ \begin{cases} 
N_{l, \theta, t_1} = \int_{t_1}^{+\infty} \ldots e^{-\int_{t_1, \theta} [\alpha_1 u_1(s, E) + \alpha_2 u_2(s, E)] \, ds} \\
N_{l, \theta, t_2} = \int_{t_2}^{+\infty} \ldots e^{-\int_{t_2, \theta} [\alpha_1 u_1(s, E) + \alpha_2 u_2(s, E)] \, ds} 
\end{cases} \]
Material decomposition

\[ N_{l, \theta} = \int_{0}^{+\infty} ... e^{-\int_{l, \theta} \mu(s, E) \, ds} \]

Not linear, but this is the only equation we have

\[ N_{l, \theta} = \int_{0}^{+\infty} ... e^{-\int_{l, \theta} \left[ \alpha_1 \mu_1(s, E) + \alpha_2 \mu_2(s, E) \right] \, ds} \]

\[
\begin{cases}
N_{l, \theta, t_1} = \int_{t_1}^{+\infty} ... e^{-\int_{l, \theta} \left[ \alpha_1 \mu_1(s, E) + \alpha_2 \mu_2(s, E) \right] \, ds} \\
N_{l, \theta, t_2} = \int_{t_2}^{+\infty} ... e^{-\int_{l, \theta} \left[ \alpha_1 \mu_1(s, E) + \alpha_2 \mu_2(s, E) \right] \, ds}
\end{cases}
\]

\[ N_{l, \theta, t} = \int_{t}^{+\infty} ... e^{-\int_{l, \theta} \sum_{m=1}^{M} \alpha_m \mu_m(s, E) \, ds} \quad t = 1, \ldots, M \]
Material decomposition

\[ N_{l, \theta} = \int_{0}^{+\infty} e^{-\int_{l,\theta} u(s, E) \, ds} \]

Not linear, but this is the only equation we have

\[ N_{l, \theta} = \int_{0}^{+\infty} e^{-\int_{l,\theta} [\alpha_1 u_1(s, E) + \alpha_2 u_2(s, E)] \, ds} \]

\[
\left\{
\begin{align*}
N_{l, \theta, t_1} &= \int_{t_1}^{+\infty} e^{-\int_{l,\theta} [\alpha_1 u_1(s, E) + \alpha_2 u_2(s, E)] \, ds} \\
N_{l, \theta, t_2} &= \int_{t_2}^{+\infty} e^{-\int_{l,\theta} [\alpha_1 u_1(s, E) - \alpha_2 u_2(s, E)] \, ds}
\end{align*}
\right.
\]

\[ N_{l, \theta, t} = \int_{t}^{+\infty} e^{-\int_{l,\theta} \sum_{m}^{M} \alpha_m u_m(s, E) \, ds} \quad t = 1, \ldots, M \]
Dual energy X-ray imaging

- No 3D information $\rightarrow$ ambiguities
- Two X-ray sources $\rightarrow$ high dose
How to really solve CT?

\[ N_{l, \theta, t} = \int_{t}^{+\infty} ... R(E, E') ... e^{-\int_{l, \theta} \sum_{m}^{M} \alpha_m u_m(s, E) \, ds} \]

1 - the threshold trick

2 - the detector response

3 - how do we invert the integral?
How to really solve CT?

\[ N_{l, \theta, t} = \int_{t}^{+\infty} \cdots R(E, E') \cdots e^{- \int_{l, \theta}^{M} \sum_{m} \alpha_{m} \mu_{m}(s, E) ds} \]

1 - the threshold trick

2 - the detector response

3 - how do we invert the integral?
Spectroscopic (hybrid) pixel detectors
Charge is proportional to energy
Charge is proportional to energy

\[ \gamma \]

\[ Q \]

\[ \gamma \]

\[ Q \]
Charge is proportional to energy

\[ Q \propto \gamma \propto \text{amplitude} \]
Energy selective photon counting
Energy selective photon counting

Single photon!
Energy selective photon counting

Threshold 1
Threshold 2
Threshold N

Single photon!
Energy selective photon counting

![Diagram of energy selective photon counting system with multiple thresholds for single photon detection.](image)

- Threshold 1
- Threshold 2
- Threshold N

Single photon!
Spectroscopic pixel readout
Spectroscopic pixel readout

CMOS technology:

- Low power
- Low noise
An example: the Medipix2 chip

- 250 nm CMOS technology
- Pixel pitch = 55 um
- 256 x 256 = 65k (active) pixels
- “Electronic noise free”
- High dynamic range (depth of the photon counter)
- 3-side tilable → larger area
- 2 simultaneous thresholds, 1 counter
An example: the Medipix2 chip

- 250 nm CMOS technology
- Pixel pitch = 55 µm
- 256 x 256 = 65k (active) pixels
- “Electronic noise free”
- High dynamic range (depth of the photon counter)
- 3-side tilable → larger area
- 2 simultaneous thresholds, 1 counter

Pixel matrix

Auxiliary logic

1.4 cm
Hybrid detectors
Hybrid detectors
Flip chip bump bonding
Typical sensors for X-ray applications:
300 um silicon
An example of CT using a Medipix-based detector

WARNING!
This is still a grayscale!

2 cm
Imaging at multiple thresholds

threshold
5 keV
Imaging at multiple thresholds

threshold 5 keV

threshold 10 keV

threshold 27 keV
A color (i.e. material resolved) CT

5 mm

COPPER

CADMIUM

PLASTIC
A color (i.e. material resolved) CT

COPPER

CADMIUM

PLASTIC
A color (i.e. material resolved) CT

5 mm

COPPER

CADMIUM

PLASTIC

photoelectric absorption [cm²/g]

Threshold 1

Threshold 2

Threshold 3

Energy [keV]
All very nice, but can you see the limitations?
How to really solve CT?

\[ N_{l, \theta, t} = \int_{t}^{+\infty} ... R(E, E') ... e^{-\int_{l, \theta}^{M} \alpha_m \mu_m(s, E) ds} \]

1 - the threshold trick

2 - the detector response

3 - how do we invert the integral?
How to really solve CT?

\[ N_{l, \theta, t} = \int_{t}^{+\infty} \ldots R(E, E') \ldots e^{-\int_{l,\theta}^{\infty} \sum_{m}^{M} \alpha_m u_m(s, E) ds} \]

1 - the threshold trick

2 - the detector response

3 - how do we invert the integral?
The energy response function

Medipix2-based silicon detector (300 um, hole collecting)
Spectral distortions due to detector effects

Incoming spectrum
Spectral distortions due to detector effects

Incoming spectrum

Detected spectrum

Charge sharing
Charge sharing
Charge sharing
Charge sharing
Charge sharing
Charge sharing

sensor

readout

$\vec{E}$
Need to study transport properties of the sensor!
Idea for an experiment

Deposit known energy at known location

Determine measured energy in same pixel
CERN test beam with 40 GeV pions

Timepix quad
Detector positioning in the beam

Side view

Top view

\[ \sim 0.5 \, ^\circ \]

\[ \sim 1 \, ^\circ \]
Energy deposit information in each pixel!
Track “cleaning” and fitting

Remove delta rays and fit
Reaching sub-pixel resolution

\[ \Delta x \sim \text{um} \]

\[ \Delta z < \text{um} \]
Measuring energy loss within pixel volume
Measuring energy loss within pixel volume

Landau distribution: energy loss in a thin sensor

\[ V = (x, y, z, E) \]
Looking at charge sharing

$z_0 = (91.5 \pm 0.9) \, \mu m$
Charge sharing at different depths

These data contain information about the shape of the charge cloud
1 – solve diffusion for an elongated distribution:

\[ Q(x, y, z) = \frac{dQ_0}{y} \delta(x - x_0) \delta(z - z_0) \]

2 – add drift under electric field

3 – fit the data!
The result: expansion of the charge cloud

From fit to experimental data
Adjusting the model parameters
Adjusting the model parameters

\[ \langle x \rangle = \sqrt{2Dt} \]
Adjusting the model parameters

\[ \langle x \rangle = \sqrt{2Dt} \]
Initial cloud size as a function of photon energy
Synchrotron test beam

European Synchrotron Radiation Facility, Grenoble, France
Synchrotron test beam

Quite unusual conditions:

- Broad beam
- Energy scan
- Adjust optics at each energy
Radiation damage

Beam spot during exposure
Radiation damage

Beam spot during exposure

Uniform irradiation after test beam
Measurement and analysis technique

Monochromatic source spectrum

Calibrated pixel spectrum
Measurement and analysis technique

Monochromatic source spectrum

Calibrated pixel spectrum

Summed pixel spectra
Measurement and analysis technique

Monochromatic source spectrum

Calibrated pixel spectrum

Now use the model
Leave $\sigma_0$ free

Summed pixel spectra
Measurement and analysis technique

Monochromatic source spectrum

Calibrated pixel spectrum

Now use the model
Leave $\sigma_0$ free

Summed pixel spectra

Fit for $\sigma_0$
Measurements and analysis technique

Monochromatic $E$ source spectrum

Calibrated pixel spectrum

Repeat for different input energies

Now use the model
Leave $\sigma_0$ free

Summed pixel spectra

Fit for $\sigma_0$
Initial cloud size as a function of photon energy
Initial cloud size as a function of photon energy
Initial cloud size as a function of photon energy
Compute monochromatic spectrum at given energy

Energy = 8 keV
Compute monochromatic spectrum at given energy

Energy = 18 keV
Compute monochromatic spectrum at given energy

Energy = 38.5 keV
Compute monochromatic spectrum at given energy
The energy response function!

\[ N_{l, \theta, t} = \int_{t}^{+\infty} \ldots \begin{bmatrix} R(E, E') \end{bmatrix} \ldots e^{-\int_{l, \theta}^{\sum M} \mu_m(s, E) ds} \]
Calculate detector spectra for any given input spectrum

Whatever input spectrum

Detector spectrum
if (chargeSharing) {
    
    R(E,E') = ⋯

} else {
    
    R(E,E') = Gauss(E,sigma);
    Conv(∫₀^+∞ dE R(E;E')I₀(E)e^{−∫₁₁₁ u(s,E)ds});

}
How to really solve CT?

\[ N_{l, \theta, t} = \int_{t}^{+\infty} ... R(E, E') ... e^{-\int_{l, \theta}^{\infty} \sum_{m}^{M} \alpha_{m} u_{m}(s, E) ds} \]

1 - the threshold trick

2 - the detector response

3 - how do we invert the integral?
How to really solve CT?

\[ N_{l, \theta, t} = \int_{t}^{+\infty} \ldots R(E, E') \ldots e^{-\int_{l, \theta}^{M} \alpha_m u_m (s, E) ds} \]

1 - the threshold trick

2 - the detector response

3 - how do we invert the integral?
Spectral computed tomography

simulation studies
Spectral CT

Motivation

- Artifact free
- Material decomposition

State of the art

- Spectroscopic pixel detectors appeared only recently
- Big companies do not disclose their progress!
Many, MANY, applications!

Functional CT

micro CT (e.g. bone tissue)

Industrial metrology

Medical CT
Inversion problem, approach #1: iterative

\[
N_{l, \theta, t} = \int_{t}^{+\infty} dE' \int_{0}^{+\infty} \ dE \ R(E; E') I_0(E) e^{-\int_{l, \theta}^{0} \sum_{m}^{M} \alpha_m u_m(s, E) ds}
\]

coefficients

unknowns
Inversion problem, approach #1: iterative

\[ N_{l, \theta, t} = \int_{t}^{+\infty} dE' \int_{0}^{+\infty} dE \, R(E; E') I_0(E) e^{-\int_{l, \theta}^{\infty} \sum_{m}^{M} \alpha_m u_m(s, E) ds} \]

1 - initial guess: \( \alpha_m^0 \)
Inversion problem, approach #1: iterative

\[ N_{l, \theta, t} = \int_t^{+\infty} dE' \int_0^{+\infty} dE \ R(E; E') \ I_0(E) e^{-\int_{l, \theta}^{s} \sum_{m}^{M} \alpha_m \ u_m(s, E) \ ds} \]

1 - initial guess: \( \alpha_m^0 \)

2 - compute image: \( N_{l, \theta, t}^0 \)
Inversion problem, approach #1: iterative

\[ N_{l,\theta,t} = \int_{t}^{+\infty} dE' \int_{0}^{+\infty} dE R(E; E') I_0(E) e^{-\int_{l,\theta}^{+\infty} \sum_{m}^{M} \alpha_m \mu_m(s,E) ds} \]

- initial guess: \( \alpha_m^0 \)
- compute image: \( N_{l,\theta,t}^0 \)
- compare: \( N_{l,\theta,t}^0 \) vs \( N_{l,\theta,t} \)
Inversion problem, approach #1: iterative

\[ N_{l, \theta, t} = \int_{t}^{+\infty} dE' \int_{0}^{+\infty} dE \ R(E; E') I_0(E) e^{-\int_{l, \theta}^{\infty} \sum_{m}^{M} \alpha_m u_m(s, E) ds} \]

1 - initial guess: \( \alpha_m^0 \)

2 - compute image: \( N_{l, \theta, t}^0 \)

3 - compare: \( N_{l, \theta, t}^0 \) vs \( N_{l, \theta, t} \)

4 - corrections: \( \epsilon_{l, \theta, t}^0 \)
Inversion problem, approach #1: iterative

\[ N_{l,\theta,t} = \int_t^{+\infty} dE' \int_0^{+\infty} dE R(E;E') I_0(E) e^{-\int_{l,\theta} \sum_m \alpha_m \mu_m(s,E) \, ds} \]

1 - initial guess: \( \alpha_m^0 \)

2 - compute image: \( N_{l,\theta,t}^0 \)

3 - compare: \( N_{l,\theta,t}^0 \) vs \( N_{l,\theta,t} \)

4 - corrections: \( \epsilon_{l,\theta,t}^0 \)

5 - update guess: \( \alpha_m^1 \)
Inversion problem, approach #1: iterative

\[
N_{l, \theta, t} = \int_t^{+\infty} dE' \int_0^{+\infty} dE \, R(E; E') I_0(E) e^{-\int_{l, \theta}^{\infty} \sum_m \alpha_m u_m (s, E) ds}
\]

1 - initial guess: \( \alpha_m^0 \)
2 - compute image: \( N_{l, \theta, t}^0 \)
3 - compare: \( N_{l, \theta, t}^0 \) vs \( N_{l, \theta, t} \)
4 - corrections: \( \epsilon_{l, \theta, t}^0 \)
5 - update guess: \( \alpha_m^1 \)

Iterate until convergence
A simulation study

Object slice

Blue = Al
Green = Ti
Red = Fe

\( \alpha_m \) (truth)
A simulation study

Object slice

Blue = Al
Green = Ti
Red = Fe

Threshold 3 keV

Threshold 10 keV

Threshold 20 keV

$\alpha_m$ (truth)

$N_{l,\theta,t}$ (dataset)
Blue = Al
Green = Ti
Red = Fe

\[ \alpha_m^0 \quad \text{(initial guess)} \]
A simulation study

\[ \alpha_0 \]

(initial guess)

\[ N_{l, \theta, t}^0 \] (computed dataset)

Blue = Al
Green = Ti
Red = Fe
A simulation study

Blue = Al
Green = Ti
Red = Fe

\[ \alpha_m^0 \] (initial guess)

\[ N_{l,\theta,t}^0 \] (computed dataset)

\[ \epsilon_{l,\theta,t}^0 \] (correction factors)
A simulation study

Blue = Al
Green = Ti
Red = Fe

\[ \alpha_{m}^{0} \quad \text{(initial guess)} \]

\[ N_{l, \theta, t}^{0} \quad \text{(computed dataset)} \]

\[ \epsilon_{l, \theta, t}^{0} \quad \text{(correction factors)} \]

\[ \alpha_{m}^{1} \]
Blue = Al
Green = Ti
Red = Fe

\[ \alpha^N_m \]
Blue = Al
Green = Ti
Red = Fe

$\alpha^N_m$

Blue = Al
Green = Ti
Red = Fe

$\alpha_m$ (truth)
Blue = Al
Green = Ti
Red = Fe

$\alpha_m^N$

$\alpha_m$ (truth)
Blue = wax
Green = Al
Red = Cu

$\alpha_m$ (truth)
Blue = wax
Green = Al
Red = Cu

$\alpha_m$ (truth)

- Divergence after few iterations
- Material space decoupled from coordinates space
Inversion problem, approach #1: statistical

\[ N_{l, \theta, t} = \int_{t}^{+\infty} dE' \int_{0}^{+\infty} dE \, R(E; E') \, I_0(E) \, e^{-\int_{l, \theta} \sum_{m}^{M} \alpha_m \mu_m(s, E) \, ds} \]
Inversion problem, approach #1: statistical

\[ N_{l, \theta, t} = \int_{t}^{+\infty} dE' \int_{0}^{+\infty} dE \ R(E; E') \ I_0(E) e^{-\int_{l, \theta}^{0} \sum_{m}^{M} \alpha_m u_m(s, E) ds} \]

Number of photons

unknowns

coefficients
Inversion problem, approach #1: statistical

\[ N_{l, \theta, t} = \int_t^{+\infty} dE' \int_0^{+\infty} dE \, R(E; E') I_0(E) e^{-\int_{l, \theta}^{l, \theta} \sum_m^M \alpha_m \mu_m(s, E) ds} \]

**coefficients**

**unknowns**

Number of photons  \(\Rightarrow\)  Poisson statistics
Inversion problem, approach #1: statistical

\[
N_{l, \theta, t} = \int_t^{+\infty} dE' \int_0^{+\infty} dE \, R(E; E') I_0(E) e^{-\int_{l, \theta}^{\infty} \sum_m^M \alpha_m \mu_m(s, E) ds}
\]

Number of photons \xrightarrow{\text{coefficients}}\ Poisson statistics

\[
P(X_{l, \theta, t} \mid N_{l, \theta, t}) = \frac{N_{l, \theta, t}^{X_{l, \theta, t}} e^{-N_{l, \theta, t}}}{X_{l, \theta, t}!}
\]
Assumption: independent variables

\[ P(X_{l,\theta,t} \mid N_{l,\theta,t}) = \frac{N_{l,\theta,t}^{X_{l,\theta,t}} e^{-N_{l,\theta,t}}}{X_{l,\theta,t}!} \]
Assumption: independent variables

\[ P( X_{l,\theta,t} | N_{l,\theta,t} ) = \frac{ N_{l,\theta,t}^{X_{l,\theta,t}} e^{-N_{l,\theta,t}} }{ X_{l,\theta,t}! } \]

\[ P( X | N ) = \prod_{l} \prod_{\theta} \prod_{t} \frac{ N_{l,\theta,t}^{X_{l,\theta,t}} e^{-N_{l,\theta,t}} }{ X_{l,\theta,t}! } \]
Assumption: independent variables

\[ P(X_1, \theta, t | N_1, \theta, t) = \frac{N_1, \theta, t^{X_1, \theta, t} e^{-N_1, \theta, t}}{X_1, \theta, t!} \]

\[ P(X | N) = \prod_l \prod_\theta \prod_t \frac{N_l, \theta, t^{X_l, \theta, t} e^{-N_l, \theta, t}}{X_l, \theta, t!} \]

Image ↔ maximum likelihood
Particle physicists are good at maximizing functions...

What do you see?
Particle physicists are good at maximizing functions...

The full Higgs combination model, 23000 functions, 1600 parameters
Image credit http://cds.nyu.edu/projects/collaborative-statistical-modeling/
... but how big is our function?

\[ N_{l, \theta, t} = 54 \times 10^3 \]

\[ N_{\text{voxels}} = 100 \times 100 = 10k \]

\[ N_{\text{materials}} = 3 \]

\[ \text{dim} \left( \text{Img} \right) = 30k \]
Particle physics vs CT likelihood

Particle physics: complex model, “few” parameters

CT: simple model, many parameters
Developing RooFit for CT at Nikhef

Nikhef
Science Park
Amsterdam
The Netherlands

W. Verkerke

me
A RooFit simulation study

- Compiling dedicated Root version
- Running on dedicated machine in the Nikhef cluster (Stoomboot)
  - 8 cores
  - 16 Gb RAM

→ $O(1 \text{ day})$ to simulate a 20 x 20 image
A RooFit simulation study

Aluminium
Iron

10 keV
4 keV
20 keV

20 keV

4 keV
10 keV
A RooFit simulation study

Aluminium image

Iron image

10 keV

4 keV

20 keV

Projection coordinate [pixel]

Angle [deg]

Projection coordinate [pixel]

Angle [deg]

Aluminium image

Iron image

voxel x

voxel y
A RooFit simulation study

Aluminium image

Iron image

10 keV

4 keV

20 keV

Coming soon:

500x500 image test on data

Aluminium image

Iron image

Projection coordinate [pixel]

Angle [deg]

Projection coordinate [pixel]

Angle [deg]
How to really solve CT?

\[ N_{l, \theta, t} = \int_{t}^{+\infty} \ldots R(E, E') \ldots e^{-\int_{l, \theta}^{+\infty} \sum_{m=1}^{M} \alpha_m u_m(s, E) ds} \]

1 - the threshold trick

2 - the detector response

3 - how do we invert the integral?
Conclusion

- Spectral CT is the future of X-ray imaging
  - possible thanks to energy sensitive pixel detectors

- Energy response function:
  - EITHER solve charge sharing (→ Medipix3)
  - OR full characterization

- Need to develop new reconstruction techniques
To download the thesis:

- The library of the University of Amsterdam: http://dare.uva.nl/record/1/432998
- The Nikhef library: http://www.nikhef.nl/pub/services/newbiblio/theses.php
- The CERN thesis database: http://cds.cern.ch/record/1971202/?ln=it

To contact me:
- enrico.junior.schioppa@cern.ch

Links:

- ctreco SVN repository: https://svnweb.cern.ch/cern/wsvn/ctreco
- My Twiki: https://twiki.cern.ch/twiki/bin/view/Main/EnricoJuniorSchioppa?forceShow=1
BACKUP
Threshold calibration with X-ray fluorescence

Photon energy $\leftrightarrow$ discriminator voltage
Threshold calibration with X-ray fluorescence

Photon energy ↔ discriminator voltage

Incident x-ray

M Shell

L Shell

K Shell

Fluorescent x-ray

* Electron

◊ Vacancy
Threshold calibration with X-ray fluorescence

Photon energy ↔ discriminator voltage

Incident x-ray

K Shell

L Shell

M Shell

Fluorescent x-ray

Electron

Vacancy

TARGET

X-RAY TUBE

PRIMARY BEAM

DETECTOR
1 - acquire 65k spectra
Threshold calibration with X-ray fluorescence

Photon energy ↔ discriminator voltage

1 - acquire 65k spectra

Typical fluorescence model has 7 parameters

1 - do 65k fits
RooFit for computed tomography: working plan

me

- Implement expectation value
- Implement probability density function (PDF)
- Simulate data
- Reconstruct

W. Verkerke

- Optimize data handling
- Identify and disable “useless” routines
- Optimize PDF handling
RooFit

RooFit v3.59 -- Developed by Wouter Verkerke and David Kirkby
Copyright (C) 2000-2013 NIKHEF, University of California & Stanford University
All rights reserved, please read http://roofit.sourceforge.net/license.txt

root [1] .q

enricojr@enricojr-Vostro-3350 ~ $
The full Higgs combination model, 23000 functions, 1600 parameters

Image credit http://cds.nyu.edu/projects/collaborative-statistical-modeling/
Some counting...

Focus on one slice only
Some counting...

Focus on one slice only

$$N_{l, \theta, t}$$
Some counting...

Focus on one slice only

\[ N_{l, \theta, t} \]
Some counting...

Focus on one slice only

\[
\begin{bmatrix}
N_{l, \theta, t} \\
100 & 180
\end{bmatrix}
\]
Some counting...

Focus on one slice only

\[ N_{l, \theta, t} \]

\[ \begin{align*} 100 & \quad 180 & \quad 3 \end{align*} \]
Some counting...

Focus on one slice only

\[ N_{l, \theta, t} = 54k \]

100 180 3
Some counting...

Focus on one slice only

$$N_{l, \theta, t} = 54k$$

$$100 \quad 180 \quad 3$$
Some counting...

Focus on one slice only

\[ N_{l, \theta, t} = 54k \]

\[ N_{\text{voxels}} = 100 \times 100 = 10k \]
Some counting...

Focus on one slice only

\[ N_{l, \theta, t} = 54k \]

\[ N_{\text{voxels}} = 100 \times 100 = 10k \]

\[ N_{\text{materials}} = 3 \]
Some counting...

Focus on one slice only

\[ N_{l, \theta, t} = 54k \]

\[ \begin{align*}
N_{\text{voxels}} &= 100 \times 100 = 10k \\
N_{\text{materials}} &= 3 \\
\text{dim}(\text{Img}) &= 30k
\end{align*} \]
High energy physics $\rightarrow$ complex models, “few” parameters
Computed Tomography $\rightarrow$ “simple” models, many parameters
Blue = Al
Green = Ti
Red = Fe

\[ \mu_m(s, E) \text{ (truth)} \]

Use big formula
Blue = Al
Green = Ti
Red = Fe

\[ \mu_m(s, E) \] (truth)

Use big formula

Threshold
3 keV
10 keV
20 keV
Blue = Al
Green = Ti
Red = Fe

$$\mu_m(s, E) \quad \text{(truth)}$$

Use big formula
Blue = Al
Green = Ti
Red = Fe

\[ \mu_m^0(s, E) \]
Blue = Al
Green = Ti
Red = Fe

$\mu_0^m(s, E)$
Blue = Al
Green = Ti
Red = Fe

\[ \mu_m^0(s, E) \]

Use big formula again
Blue = Al
Green = Ti
Red = Fe

\[ \mu_m(s, E) \]

Threshold 3 keV
Threshold 10 keV
Threshold 20 keV
Blue = Al
Green = Ti
Red = Fe

\[ \mu_m^0(s, E) \]
Blue = Al
Green = Ti
Red = Fe

\[ \mu_{m}^{0}(s, E) \]

\[ \mu_{m}^{1}(s, E) \]
Calculating charge fraction in a pixel

Charge cloud

Pixels (top view)
Calculating charge fraction in a pixel
Calculating charge fraction in a pixel

$z = 7 \, \mu m$
Calculating charge fraction in a pixel

\[ z = 60 \, \mu m \]
Input spectrum
Input spectrum

Charge sharing
Input spectrum

Charge sharing

Si absorption curve
Input spectrum

Charge sharing

Si absorption curve
Timepix calibration

Calibration of the Timepix energy scale
~ roughly 1 week of work
Single threshold vs energy window

\[
\begin{align*}
N_{l, \theta, t_1} &= \int_{t_1}^{+\infty} \cdots e^{-\cdots} \\
N_{l, \theta, t_2} &= \int_{t_2}^{+\infty} \cdots e^{-\cdots}
\end{align*}
\]
Single threshold vs energy window

\[
\begin{align*}
N_{l, \theta, t_1} &= \int_{t_1}^{+\infty} \ldots e^{\ldots} \\
N_{l, \theta, t_2} &= \int_{t_2}^{+\infty} \ldots e^{\ldots}
\end{align*}
\]

\[
\begin{align*}
N_{l, \theta, t_{12}} &= \int_{t_1}^{t_2} \ldots e^{\ldots} \\
N_{l, \theta, t_{23}} &= \int_{t_2}^{t_3} \ldots e^{\ldots}
\end{align*}
\]
Single threshold vs energy window

\[
\begin{align*}
N_{l, \theta, t_1} &= \int_{t_1}^{+\infty} \cdots e^{-\cdots} \\
N_{l, \theta, t_2} &= \int_{t_2}^{+\infty} \cdots e^{-\cdots}
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\]

\[
\begin{align*}
N_{l, \theta, t_{12}} &= \int_{t_1}^{t_2} \cdots e^{-\cdots} \\
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\end{align*}
\]
Single threshold vs energy window

\[
\begin{align*}
N_{l, \theta, t_1} &= \int_{t_1}^{+\infty} \ldots e\cdots \\
N_{l, \theta, t_2} &= \int_{t_2}^{+\infty} \ldots e\cdots \\
N_{l, \theta, t_{12}} &= \int_{t_1}^{t_2} \ldots e\cdots \\
N_{l, \theta, t_{23}} &= \int_{t_2}^{t_3} \ldots e\cdots
\end{align*}
\]
\[ I_{l,\theta} = I_0 e^{-\int_{l,\theta} \mu(s) \, ds} \]

\[ \int_{l,\theta} \mu(s) \, ds = -\log \frac{I_{l,\theta}}{I_0} \]

Linear system!

\[ I_{l,\theta}(E) = I_0(E) e^{-\int_{l,\theta} \mu(s,E) \, ds} \]
\[ I_{l,\theta} = I_0 e^{-\int_\theta^l \mu(s) ds} \]

\[ \int_\theta^l \mu(s) ds = -\log \frac{I_{l,\theta}}{I_0} \]

Linear system!

\[ I_{l,\theta}(E) = I_0(E) e^{-\int_\theta^l \mu(s,E) ds} \]
\[ I_{l,\theta} = I_0 e^{-\int_{l,\theta} \mu(s)ds} \]
\[ I_{l,\theta} = I_0 e^{-\int_{l,\theta} \mu(s) \, ds} \]

\[ \int_{l,\theta} \mu(s) \, ds = -\log \frac{I_{l,\theta}}{I_0} \quad \text{Linear system!} \]

\[ I_{l,\theta}(E) = I_0(E) e^{-\int_{l,\theta} \mu(s,E) \, ds} \]

![Energy spectra](energy_spectra.png)
\[ I_{l,\theta} = I_0 e^{-\int_{l,\theta} \mu(s) ds} \quad \Rightarrow \quad \int_{l,\theta} \mu(s) ds = -\log \frac{I_{l,\theta}}{I_0} \]

Linear system!

\[ I_{l,\theta}(E) = I_0(E) e^{-\int_{l,\theta} \mu(s,E) ds} \]

Still doable, BUT...
\[ I_{l, \theta} = I_0 e^{\int_{l, \theta} \mu(s) ds} \]

\[ \int_{l, \theta} \mu(s) ds = -\log \frac{I_{l, \theta}}{I_0} \quad \text{Linear system!} \]

\[ I_{l, \theta}(E) = I_0(E) e^{\int_{l, \theta} \mu(s, E) ds} \]

\[ N_{l, \theta} = \int_{0}^{+\infty} dE I_{l, \theta}(E) \]

Still doable, BUT...
\[ I_{l, \theta} = I_0 e^{-\int_{l, \theta} \mu(s) \, ds} \]

\[ \int_{l, \theta} \mu(s) \, ds = -\log \frac{I_{l, \theta}}{I_0} \]

Still doable, BUT...

\[ I_{l, \theta}(E) = I_0(E) e^{-\int_{l, \theta} \mu(s, E) \, ds} \]

\[ N_{l, \theta} = \int_{0}^{+\infty} dE \, I_{l, \theta}(E) \]

\[ N_{l, \theta} = \int_{0}^{+\infty} dE \, I_0(E) e^{-\int_{l, \theta} \mu(s, E) \, ds} \]
\[ I_{l,\theta} = I_0 e^{-\int_{l,\theta} \mu(s) ds} \]

\[ \int_{l,\theta} \mu(s) ds = -\log \frac{I_{l,\theta}}{I_0} \]

Linear system!

\[ I_{l,\theta}(E) = I_0(E) e^{-\int_{l,\theta} \mu(s, E) ds} \]

Still doable, BUT...

\[ N_{l,\theta} = \int_0^{+\infty} dE \ I_{l,\theta}(E) \]

\[ N_{l,\theta} = \int_0^{+\infty} dE \ I_0(E) e^{-\int_{l,\theta} \mu(s, E) ds} \]
\[ N_{l, \theta} = \int_{0}^{+\infty} dE \ I_0(E) e^{-\int_{l, \theta} \mu(s, E) ds} \]
\[ N_{l, \theta} = \int_{0}^{+\infty} dE \ I_0(E) \ e^{-\int_{l, \theta} \mu(s, E) \ ds} \]

\[ I(E) \]

A tube spectrum after transmission through the sample
\[ N_{l, \theta} = \int_{0}^{+\infty} dE \ I_0(E) e^{-\int_{l, \theta} \mu(s, E) ds} \]

\[ I(E) \]

A tube spectrum after transmission through the sample

A tube spectrum as seen by a Medipix2-based silicon detector
OBJECT $\mu(x,y,z)$

SECTION $\mu(x,y)$

BEAM
X-RAY PATH $r, \theta$

COORDINATE ALONG THE X-RAY PATH

COORDINATE IN THE DETECTOR PLANE
\[ I_{l,\theta} = I_0 e^{-\int_{l,\theta} \mu(s) ds} \]
\[ I_{l,\theta} = I_0 e^{-\int_{l,\theta} \mu(s) ds} \]

\[ \int_{l,\theta} \mu(s) ds = -\log \frac{I_{l,\theta}}{I_0} \]

A linear system, can you see it?
PIXEL = PIconut EEléments

VOXEL = 3D pixel

detector

image
backprojection
backprojection
backprojection
RULE #5 (the most important!): 
NEW RECONSTRUCTION ALGORITHM
\[ N = N_0 e^{-\int_L \mu(x) dx} \]
\[ N = N_0 e^{-\int_L \mu(x) \, dx} \]
\[ N = N_0 e^{-\int L \mu(x) dx} \]

\[ N(E) = N_0(E) e^{-\int L \mu(x, E) dx} \]
\[ N(E) = N_0(E) e^{-\int_{L_1} \mu_1(x, E) \, dx - \int_{L_2} \mu_2(x, E) \, dx} \]
\[
N(E) = N_0(E) e^{-\int_{L_1}^{L_2} \mu_1(x, E) dx - \int_{L_2}^{} \mu_2(x, E) dx}
\]
RULE #1:
ENERGY (COLOR) = MATERIAL

\[ N(E) = N_0(E)e^{-\int_{L_1}^{L_2} \mu_1(x, E)dx - \int_{L_1}^{L_2} \mu_2(x, E)dx} \]
\[ N = \int_{0}^{+\infty} dE N_0(E) e^{-\int_{L_1} \mu_1(x,E) dx - \int_{L_2} \mu_2(x,E) dx} \]
RULE #2:
NEED TO GO
+ density!
Computed Tomography (CT)
Computed Tomography (CT)
Some brain missing?

What the heck is going on here?
BEAM HARDENING
BEAM HARDENING

source

detector

$E$
Beam Hardening

source

detector

$E$

$E$
BEAM HARDENING

detector

source

$E$

$E$

$E$
RULE #3: NEED TO MEASURE ENERGY
Hybrid pixel detectors
Medipix

- 256 x 256 = 64k (active) pixels
- Pixel pitch = 55 um
- Electronic noise free
- High dynamic range (depth of the photon counter)
- 3-side tilable → larger area
- Up to 8 simultaneous thresholds
Medipix

- 256 x 256 = 64k (active) pixels
- Electronic noise free
- High dynamic range (depth of the photon counter)
- 3-side tilable → larger area
- Up to 8 simultaneous thresholds

RULE #4: #materials = #thresholds
Conventional = monochromatic approximation
Conventional = monochromatic approximation

\[ N = N_0 e^{-\int L \mu(x) dx} \]
Conventional = monochromatic approximation

\[ N = N_0 e^{- \int_L \mu(x) \, dx} \quad \Rightarrow \quad - \int_L \mu(x) \, dx = \log \frac{N}{N_0} \]
Conventional = monochromatic approximation

\[ N = N_0 e^{-\int_L \mu(x) \, dx} \]

\[ -\int_L \mu(x) \, dx = \log \frac{N}{N_0} \]

\[ N = \int_0^{+\infty} dE \, N_0(E) e^{-\int_L \mu(x, E) \, dx} \]
\[ N_{l\theta}^{thr} = \int_{0}^{+\infty} dE \mathcal{N}(E) e^{-\int_{x}^{L} \mu(x, E) dx} \]

WHATEVER COMPLICATED INTEGRAND
This number obeys Poisson statistics

\[ N_{\theta \text{ thr}} = \int_0^{+\infty} \text{d}E N_0(E) e^{-\int \mu(x, E) \text{d}x} \]

\[ P(X_{1\theta}^{\text{thr}} \mid N_{1\theta}^{\text{thr}}) = \frac{N_{1\theta}^{\text{thr}} X_{1\theta}^{\text{thr}}}{X_{1\theta}^{\text{thr}}} e^{-N_{1\theta}^{\text{thr}}} \]

WHATEVER COMPLICATED INTEGRAND
This number obeys Poisson statistics

\[ N_{l\theta}^{thr} = \int_{0}^{+\infty} dE \]

\[ P \left( X_{l\theta}^{thr} \mid N_{l\theta}^{thr} \right) = \frac{N_{l\theta}^{thr} X_{l\theta}^{thr} e^{-N_{l\theta}^{thr}}}{X_{l\theta}^{thr}!} \]

\[ P \left( X \mid N \right) = \prod_{l \theta \ thr} \frac{N_{l\theta}^{thr} X_{l\theta}^{thr} e^{-N_{l\theta}^{thr}}}{X_{l\theta}^{thr}!} \]
$$N_{l\theta}^{thr} = \int_{E_{l}^{thr}}^{\infty} dE \int_{0}^{\infty} dE' \ R(E;E') \ S_{0}(E) e^{-\sum_{n} \rho_{n} \frac{\mu_{n}(E)}{\rho_{n}} \int_{l\theta} f_{n}(x) dx}$$
\[ N_{l\theta}^{thr} = \int_{E_l^{thr}}^{\infty} dE \int_{0}^{\infty} dE' R(E; E') S_0(E) e^{-\sum_n \frac{\mu_n}{\rho_n}(E) \int_{l\theta} f_n(x) dx} \]
\[ N_{l\theta}^{thr} = \int_{E_l^{thr}}^{\infty} dE \int_{0}^{\infty} dE' R(E; E') S_0(E) e^{-\sum \rho_n \frac{\mu_n(E)}{\rho_n} \int_{l\theta} f_n(x) dx} \]
\[ N_{l\theta}^{\text{thr}} = \int_{E_{l}^{\text{thr}}}^{\infty} dE \int_{0}^{\infty} dE' R(E; E') S_0(E) e^{-\sum \rho_n \mu_n(E) \int_{l\theta} f_n(x) dx} \]

(measured) source spectrum

Detector response function

(known) absorption coefficients + (nominal) densities

(measured) densities (known) source spectrum
\[ N_{\theta}^{thr} = \int_{E_{thr}^l}^{\infty} dE \int_{0}^{\infty} dE' R(E; E') S_0(E) e^{-\sum \rho_n \frac{\mu_n(E)}{\rho_n} \int_{l_0} f_n(x) dx} \]
\[ N_{l\theta}^{\text{thr}} = \int_{E_l^{\text{thr}}}^{\infty} dE \int_{0}^{\infty} dE' R(E; E') S_0(E) e^{-\sum \frac{\mu_n(E)}{\rho_n(E)} \int_{1\theta} f_n(x) dx} \]

Detector response function

(measured) source spectrum

(measured) absorption coefficients + (nominal) densities

Vector image

\[
P(X|N) = \prod_{l\theta \text{thr}} \frac{N_{l\theta}^{\text{thr}} X_{l\theta}^{\text{thr}} e^{-N_{l\theta}^{\text{thr}}}}{X_{l\theta}^{\text{thr}} !}
\]
\[ N_{l\theta}^{thr} = \int_{E_l^{thr}}^{\infty} dE \int_{0}^{\infty} dE' R(E; E') S_0(E) e^{-\sum_{n} \rho_n \mu_n(E) \int f_n(x) dx} \]

Detector response function

\[ f_n(x) = \arg\max P(X|N) = \arg\max \prod_{l\theta} N_{l\theta}^{thr} X_{l\theta}^{thr} e^{-N_{l\theta}^{thr}} X_{l\theta}! \]
Probability density function

Poisson 1  Poisson 2  Poisson 3  \ldots  Poisson N
Probability density function

\[ N_{\text{parameters}} = N_{\text{voxels}}^2 \times N_{\text{materials}} \]

\[ N_{\text{data}} = N_{\text{pixels}} \times N_{\text{angles}} \times N_{\text{thresholds}} \]
Probability density function

\[ N_{\text{parameters}} = N_{\text{voxels}}^2 \times N_{\text{materials}} \]

\[ N_{\text{data}} = N_{\text{pixels}} \times N_{\text{angles}} \times N_{\text{thresholds}} \]
The full Higgs combination model, 23000 functions, 1600 parameters
Image credit http://cds.nyu.edu/projects/collaborative-statistical-modeling/
Nikhef
Science Park
Amsterdam
The Netherlands

W. Verkerke

me
Next steps:

- Optimize RooFit:
  - High energy physics $\rightarrow$ complex models, “few” parameters
  - Computed Tomography $\rightarrow$ “simple” models, many parameters
- Test on data
- Test on biological materials
### LAST MODIFICATION

**Rev 16 2015-02-16 19:00:43**

**Author:** idarraga  

**Log message:** checking that the OB file exists and is not full of zeroes

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Summary: the 5 rules

RULE #1: ENERGY (COLOR) = MATERIAL

RULE #2: NEED TO GO

RULE #3: NEED TO MEASURE ENERGY

RULE #4: #materials = #thresholds

RULE #5: NEW RECONSTR. ALGORITHM